Escuela Politécnica Superior

Economic feasibility study of the heat integration of an i-butane/n-butane mixture distillation process

Grado en Ingeniería Química

Trabajo Fin de Grado

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Index

Abstract

A 100 kmole/h i-butane/n-butane mixture was selected to analyze the feasibility of heat integration of a conventional distillation process using mechanical heat pumps and multiple effect distillation.

The conventional distillation column as well as the top vapor recompression and bottom flashing heat pumps and the multiple effect distillation process were simulated using the HYSYS software to determine the best economical alternative.

The top vapor recompression heat pump and the bottom flashing one reduce the global utility consumption by 86% and 87% respectively, but due to the utility cost difference the yearly operating cost is only reduced by 50% and 54%. However, the annualized capital cost of the equipment is increased by 121% for the top vapor recompression and 71,4% for the bottom flashing one reducing the Equivalent Annual Operating Cost only by 13% and 27%.

The results are more favorable in case of the multiple effect distillation, reducing the energy consumed by 50% and the operating cost by 55%, with only increasing the initial capital investment by 20%. Reducing the EAOC by 39% this way.

Key words

Distillation, optimization, heat integration, heat pump, energy savings, simulation, capital-equipment cost, module factor approach

Greetings

To my parents Lola Vélez Campos and Enrique Sirera Contreras

for never losing faith in me in all these years.

To my beloved Anacaona for her unconditional support.

And to all the magnificent teachers of the “Universidad de Alicante” for opening me the doors of the ever-growing world of the chemical engineering and transmitting me their passion with their hard work.

To all the members of Applynano solutions. I have learnt a lot from them, and they are magnificent people.

List of nomenclature

Abbreviations

Symbol	Definition	Units
AEC	Annualized Equipment Cost	€/year
C	Cost	€
Fq	Quantity Factor	
CEPCI	Chemical Engineering Plant Cost Index	
D	Diameter	m
EAOC	Equivalent Annual Operating Cost	€/year
F_P	Pressure Factor	
N	Number of Trays	
P	Pressure	kPa, barg
R	Reflux Ratio	
YOC	Yearly Operative Cost	€/year
yr	Year	year
CD	Conventional Distillation	
TVRHP	Top Vapor Recompression Heat Pump	
BFHP	Bottom Flashing Heat Pump	
MED	Multiple Effect Distillation	
F_M	Material Factor	
F_{BM}	Bare Module Factor	
C_p^o	Purchased Equipment Cost	$, €

Greek symbols

ΔT	Temperature Difference	^oC, K
Ln	Natural Logarithm	

Subscripts

1	Base Time, Base Case or Inlet Condition
2	Desired Time, New Case or Outlet Condition
C	Condenser
R	Reboiler
C-R	Between Condenser and Reboiler
min	Minimum
BM	Bare Module
I	Inner
O	Outer
LM	Logaritmic Mean
tot	Total

References

[1] B. Linhoff, H. Dunford, R. Smith. Heat Integration of Distillation Columns into Overall Processes. Chemical Engineering Science. Pergamon Press. (1983)

[2] Aspentech HYSYS Web: https://www.aspentech.com/en/products/engineering/aspen-hysys

[3] R, Turton. *Analysys Synthesis an Design of Chemical Processes.* Prentice Hall. (2018).

[4] K.M. Guthrie, *Process Plant Estimating Evaluation and Control.* Craftsman Book Co. (1974).

[5] G. D. Ulrich, *A Guide to Chemical Engineering Process Design and Economics.*

[6] K.E. Herold. Absorption Chillers and Heat Pumps.CRC Press. (2016)

[7] J.M. Coulson, J.F. Richardson, Chemical Engineering, vol. 6, Pergamon Press, Oxford, 1993. pp. 565–702.

[8] Chemical Engineering Web: https://www.chemengonline.com

[9] D.W. Green, R.H. Perry. Perry's Chemical Enigineer's Handbook. McGraw-Hill. 2008)

[10] Tubular Exchanger Manufacturers Association (TEMA). Standards of the Tubular Exchanger Manufacturers Association. Tubular Exchanger Manufacturers Association. (2013)

[11] D.E. Garret. Chemical Engineering Economics. (1989)

DOCUMENT I.
MEMORY

1. Background

Distillation is a highly energy consuming process. The need to provide large amounts of energy to the bottom stream and to subtract it form the top, translates into an elevate operating and environmental cost. Energy integration is key to mitigate this issue and increase the competitivity of the process.

"*Distillation is the most widely used separation process in the chemical industry. It is also a highly energy-intensive unit operation, with some processes consuming a third or more of their energy in distillation alone. It is thus a prime target for ehergy conservation*."[1]

In a heat integration process, the temperatures of the streams involved are required to be lined up favorably when entering and leaving the heat exchanger. However, in this project, an equimolar mixture of i-butane and n-butane has been chosen for its components' close boiling point. Resulting in a small temperature gap between hot and cold stream and an insufficient heat flow, increasing the complexity of the heat exchange's design procedure. To achieve feasible heat integration conditions those streams properties ought to be modified to more suitable ones. For this purpose, mechanical heat pumps are used, meeting the needs for an optimal heat exchange between the top and the bottom streams. And, between the wide variety of different heat pumps that could be applied, the top vapor recompression heat pump and the bottom flashing heat pumps are the chosen candidates.

In case of the multiple effect distillation the streams leave the distillation columns in the right conditions to achieve a feasible heat exchange, and therefore there is no need to modify them, so they enter directly the heat exchanger.

2. Objective

The objective of this work is to study the economic feasibility of a heat integration process added to a distillation column to reduce the total cost, (sum of the equipment and operative costs) in a ten-year period. Doing a Major Equipment Estimate.

To do so the cost of the distillation column without heat integration is compared with a process that uses an optimized top vapor recompression heat pump and an alternative one that uses a bottom flashing heat pump. Also, taking a different approach, the possibility of substituting the conventional distillation column with a multiple effect distillation disposal was studied.

All process data is obtained by simulating the processes in Aspen HYSYS version 10[2]. And all equipment costs are calculated using the module factor approach as explained by Turton[3] that was originally introduced by Guthrie[4] and modified by Ulrich[5].

3. Conventional distillation of an i-butane/n-butane mixture

3.1 Characteristics of the chosen mixture

Isobutane or 2-methyl propane is an alkane obtained by isomerization of n-butane (butane). This isomer is used as refrigerant or, in refineries and alkylation units, to synthetize isooctane. Isooctane is rated at 100 points on the octane rating and therefore it is blended with other hydrocarbons to improve the ani-knock properties of gasoline, more suitable for high-performance gasoline engines.

2-metylpropane has a standard boiling point of -6,945 (ºC) versus -0,7350 (ºC) of the butane.

This small boiling point difference and the fact that the mixture has no azeotropes in the desired working pressure range (500 kPa to 1000 kPa) makes conventional distillation suitable as a separation method.

3.2 HYSYS simulation of the conventional distillation column

Peng Robinson's property package has been chosen because it has been proven suitable for the prediction of the equilibrium of light hydrocarbon mixtures, like i-butane/n-butane, in the past.

3.3 Distillation conditions

The system is fed with a saturated liquid stream of 100 kmole/h of an equimolar mixture of i-butane and n-butane. Then it is separated into a saturated liquid stream of 50 kmoles/h with a molar faction of 0,9 i-butane and 10% n-butane leaving the top of the conventional column. And a bottom stream of saturated liquid with a molar flow of 50 kmoles/h and a molar fraction of 0,1 i-butane and 0,9 of n-butane.

3.4 Number of stages and columns simulation

Firstly, the Shortcut method is used to determine the actual number of stages and the optimal feed stage. In this method the independent variables are the feed stream conditions as well as the reflux ratio.

For the feed stream conditions temperature, molar flow and composition are fixed and the pressure is varied between 510 kPa and 1010 kPa. In this way, considering a total pressure drop of 20 kPa for all cases, the top pressure will vary from 500 kPa to 1000 kPa with an increment of 100 kPa. The lower value is 500 kPa because the top temperature is the minimum allowable to use water as cooling fluid in the condenser. The reflux ratio is calculated multiplying the minimum reflux ratio per R/R_{min} coefficient, in a range from 1,1 to 1,2 and an increase of 0,1. The results are shown in table 3.4.1.

Table3.4.1. Number of trays and optimal feed stage for every studied combination of pressure and reflux ratio.

	500 kPa		600 kPa		700 kPa		800 kPa		900 kPa		1000 kPa	
R/Rmin	Actual Number of Trays	Optimal Feed Stage	Actual Number of Trays	Optimal Feed Stage	Actual Number of Trays	Optimal Feed Stage	Actual Number of Trays	Optimal Feed Stage	Actual Number of Trays	Optimal Feed Stage	Actual Number of Trays	Optimal Feed Stage
1,1	39	20	41	21	43	22	45	23	47	24	49	25
1,2	33	17	35	18	37	19	39	20	40	20	42	21
1,3	30	15	32	16	33	17	35	18	36	18	38	19
1,4	28	14	30	15	31	16	32	16	34	17	35	18
1,5	26	13	28	24	29	15	31	16	32	16	33	17

In second place, the distillation columns are simulated using the different pressures and the number of trays corresponding to the reflux ratio for every case. Specifying the composition in the condenser as molar fraction of n-butane (heavy) equal to 0,1; and the composition in the reboiler as molar fraction of i-butane (light). The objective is to determine the best alternative comparing the Equivalent Annual Operating Costs, tables 3.5.1 and 3.5.2.

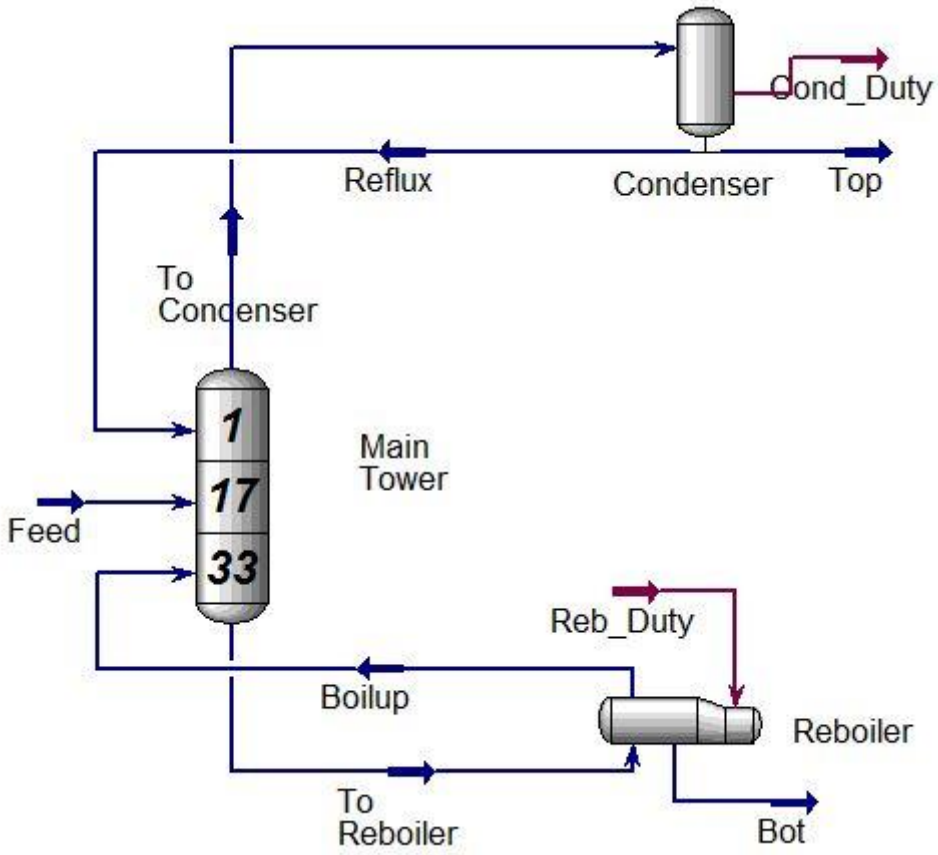

Figure 3. 4. 1. Process Flow Diagram of the Standard Distillation.

Table 3.4.2. Data from streams of the simulation of the conventional column working at 700 kPa and a reflux rate of 1,3 times the minimum rate.

	Unit	Feed	To Condenser	Top	Reflux	To Reboiler	Bottom	Boilup
Vapour Fraction		0	1	0	0	0	0	1
Temperature	*ºC*	57,69	52,54	52,24	52,24	63,34	63,65	63,65
Pressure	*kPa*	710	700	700	700	720	720	720
Molar Flow	*kgmole/h*	100	404,5	50,0	354,5	437,4	50,0	387,4
Mass Flow	*kmol/h*	5812	23513	2906	20607	25421	2906	22515
Mole Frac (i-Butane)		0,5	0,9000	0,9000	0,9000	0,1220	0,1000	0,1248
Mole Frac (n-Butane)		0,5	0,1000	0,1000	0,1000	0,8780	0,9000	0,8752
Heat Flow	*kW*	-4063	-14851	-2080	-14751	-17358	-1982	-13395

3.5 Heat integration alternatives

Looking at table 3.5.1 it is easy to perceive that the operating cost is twice or even three times higher than the annualized cost. To optimize this process the heat integration is key.

Three alternatives are used: a top vapor recompression heat pump, a bottom flashing heat pump and a multiple effect distillation instead of the conventional distillation.

Table 3.5.1. Results of simulation of conventional distillation using different top pressures at a reflux ratio of 1.3 times the minimum.

R/R_{min} = 1,3				
Top Pressure (kPa)	**EAOC (€/yr)**	**AEC (€/yr)**	**YOC (€/yr)**	**Power Consumed (kJ/h)**
500	$3{,}542 \cdot 10^5$	$8{,}941 \cdot 10^4$	$2{,}647 \cdot 10^5$	$1{,}336 \cdot 10^7$
600	$3{,}589 \cdot 10^5$	$8{,}739 \cdot 10^4$	$2{,}715 \cdot 10^5$	$1{,}366 \cdot 10^7$
700	$3{,}680 \cdot 10^5$	$8{,}441 \cdot 10^4$	$2{,}836 \cdot 10^5$	$1{,}427 \cdot 10^7$
800	$3{,}845 \cdot 10^5$	$9{,}603 \cdot 10^7$	$2{,}885 \cdot 10^5$	$1{,}461 \cdot 10^7$
900	$4{,}071 \cdot 10^5$	$1{,}018 \cdot 10^5$	$3{,}053 \cdot 10^5$	$1{,}520 \cdot 10^7$
1000	$4{,}105 \cdot 10^5$	$1{,}077 \cdot 10^5$	$3{,}027 \cdot 10^5$	$1{,}607 \cdot 10^7$

Table 3.5.2. Results of simulation of conventional distillation using different reflux ratios for a top pressure of 700 kPa.

Top Pressure (kPa) = 700				
R/R_{min}	**EAOC (€/yr)**	**AEC (€/yr)**	**YOC (€/yr)**	**Power Consumed (kJ/h)**
1,1	$3{,}422 \cdot 10^5$	$9{,}353 \cdot 10^4$	$2{,}487 \cdot 10^5$	$1{,}251 \cdot 10^7$
1,2	$3{,}565 \cdot 10^5$	$9{,}195 \cdot 10^4$	$2{,}646 \cdot 10^5$	$1{,}331 \cdot 10^7$
1,3	$3{,}680 \cdot 10^5$	$8{,}441 \cdot 10^4$	$2{,}836 \cdot 10^5$	$1{,}427 \cdot 10^7$
1,4	$3{,}901 \cdot 10^5$	$9{,}275 \cdot 10^4$	$2{,}974 \cdot 10^5$	$1{,}496 \cdot 10^7$
1,5	$4{,}105 \cdot 10^5$	$9{,}414 \cdot 10^4$	$3{,}163 \cdot 10^5$	$1{,}592 \cdot 10^7$

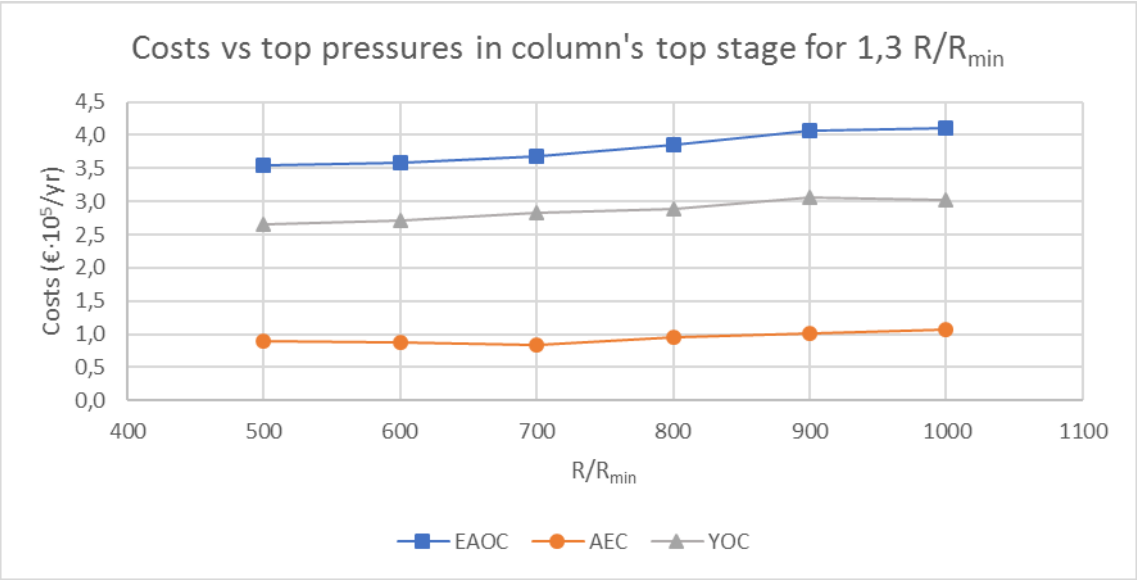

Figure 3.5.1. Annualized costs of the Conventional Distillation process of i-butane/n-butane mixture, working at 1.3 times the minimum reflux ratio at different pressures.

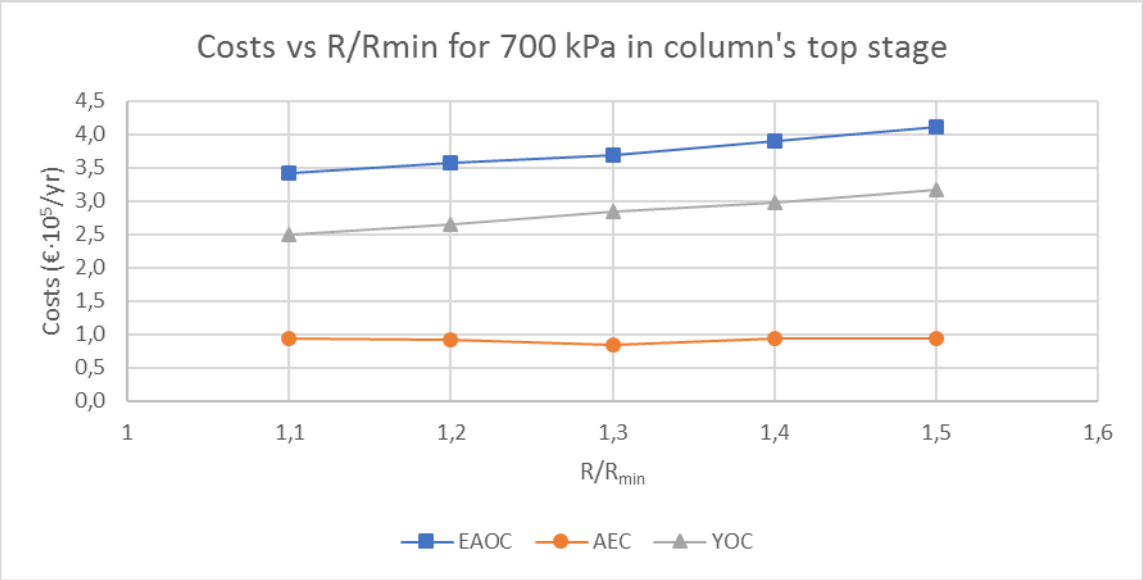

Figure 3.5.2. Annualized costs of the Conventional Distillation process of i-butane/n-butane mixture, working at 700 kPa with different reflux ratios.

4 Heat pumps

"The term "heat pump" refers to a group of technologies that transfer heat from a low temperature to a high temperature. Such technologies include refrigeration systems as well as heat pump heating systems. Such a transfer requires a thermodynamic input in the form of either work or heat. This is made clear in the Clausius statement of the Second Law of thermodynamics:

> *It is impossible for any system to operate in such a way that the sole result would be an energy transfer by heat from a cooler to a hotter body."*[6]

4.1 Compression heat pumps

The thermic cycle of a mechanic heat pump in traduces energy to the system in form of work to rise the temperature enough to be dissipated in the condenser. There the pressure and the temperature diminish. Later, energy is provided in the evaporator to vaporize the fluid which enters again in the compressor.

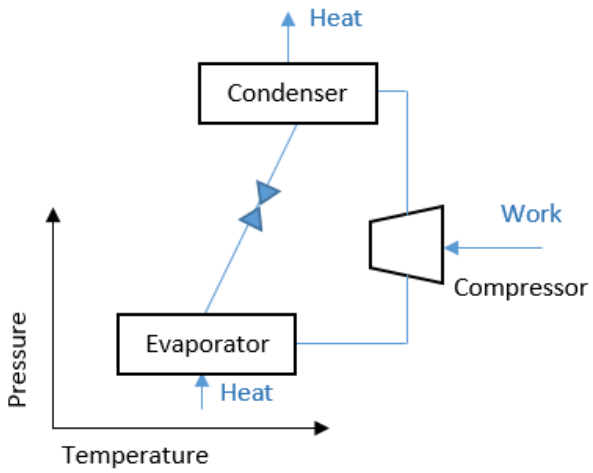

Figure 4.1. Vapor compression heat pump.

The distillation column working at steady state is not very different from said cycle, therefore the principles of the heat pump can be applied. When the bottom and the top streams are connected using a heat pump the system can be divided in to two sub cycles.

In the case of the top vapor recompression heat pump the top sub cycle is the one containing the heat pump. Starting with the stream leaving the top of the column that enters the compressor. The heat exchanger connecting the top and the bottom streams acts as the condenser and then the column acts as evaporator. Closing the sub cycle with the stream leaving the top of the column.

The bottom flashing heat pump cycle is placed in the second cycle. The stream leaving the bottom of the column enters a valve reducing the temperature and the pressure. Then enters the heat exchanger that acts as evaporator. The vapor is compressed to rise its temperature and pressure and enters the column where it condenses and leaves through the bottom closing the energy cycle.

4.1.1 Simulation of the top vapor recompression heat pump

In the distillation with top vapor recompression heat pump, the top stream temperature is raised by the compressor (K-100) to reach a high enough temperature to vaporize the same amount of mixture as the simulated in the reboiler stream of the previously simulated conventional distillation. Then the stream enters the heat exchanger, simulated in this case as a cooler and a heater sharing the energy stream, see figure 4.1.1.

An adjust was used to set the pressure of the stream leaving the compressor so that the minimum approach in the heat exchanger was 5 (ºC)[7]. This value is typical for this type of heat exchanger to achieve a balance between operational and capital cost. Further research could be required to fully optimize this part of the process. Setting the pressure, the duty of the compressor is calculated by HYSY and therefore the electricity required in such crucial part of the cycle.

After leaving the heat exchanger the cold stream (Bot2_TVRHP) is at the right temperature and pressure to be introduced in the bottom as reboiled stream. However, the stream is a mixture of gas and liquid that needs to be introduced in a separator (V-100) were the vapor leaves the top in the same conditions as in the boilup of the conventional distillation column and in the bottom 50 kmole/h of n-butane 90% purity leave the process.

On the other hand, the hot stream (Top2_TVRHP) leaves the heat exchanger at very high pressure and temperature, a water cooler (E-100) and an expansion valve (VLV-100) are used to lower this values down to the ones obtained in the reflux of the conventional distillation. Finally, 50 kmoles/h of i-butane with a 90% purity are splat from the process as product (Top_TVRHP).

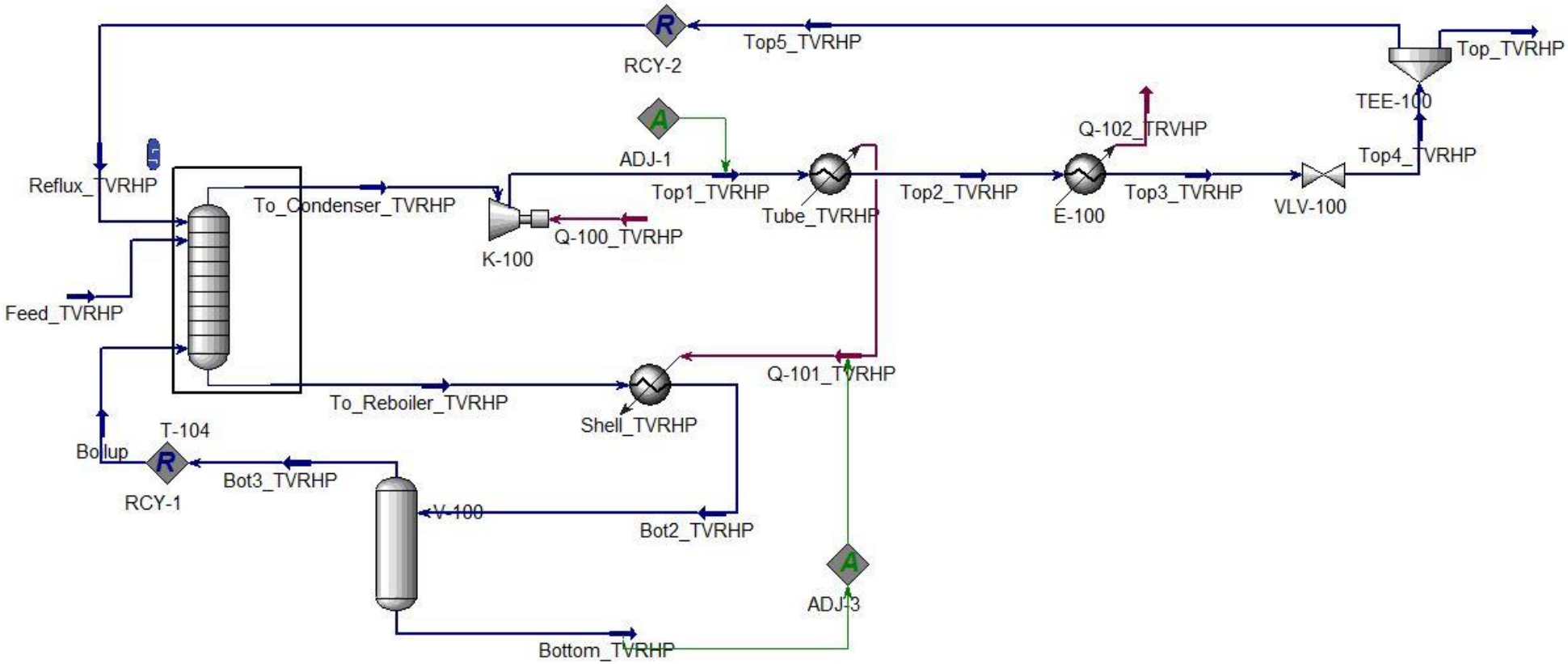

Figure 4.4.1. Bottom Flashing Heat Pump process flow diagram.

4.1.2 Simulation of the bottom flashing heat pump

For the bottom flashing heat pump the feed stream has the same characteristics as the conventional distillation. The column is simulated using an absorber (T-104). The reflux and the boilup entering the column are defined with the data obtained from the ones belonging to the conventional distillation column. The steam leaving the column's bottom enters an expansion valve (VLV-101) to reduce its temperature enough to be heated by the distillate leaving the top of the column (To_Condenser_BFHP). An adjust is used to set the pressure drop at a value that allows the heat exchanger to vaporize all the bottom stream while condensing all the vapor in the top. This condensed vapor (Top1_BFHP), once subtracted 50 kmol/h has the same conditions of the reflux, enabling the close of the recycle (RCY-2). The vaporized liquid leaving the heat exchanger (Bot2_BFHP) is at a lower pressure and temperature compared with the boilup required ones. Therefore, is introduced in a compressor (K-100). The pressure now corresponds with the boilup, but the temperature is slightly higher, a water cooler (E-100) reduces the temperature to the right one, condensing part of the mixture (Bot4_BFHP). The stream enters a separator (V-100) were the vapor is reintroduced to the column as boilup (Boilup) and the liquid, 50 kmol/h of n-butane 90% of purity, is splat form the process.

Previously mentioned streams and equipment reference the ones shown in figure 4.4.2

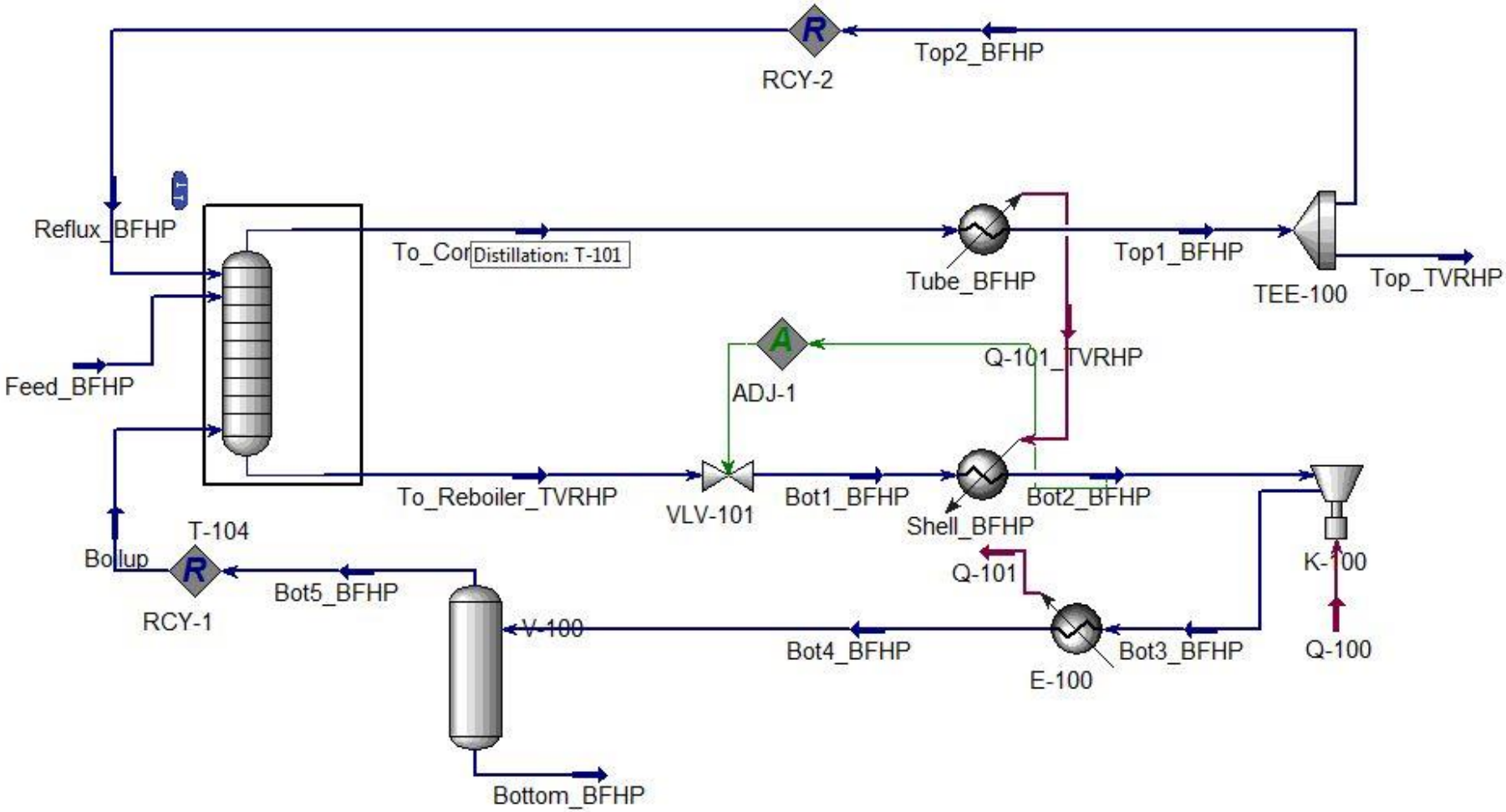

Figure 4.4.2. Bottom Flashing Heat Pump process flow diagram.

5 Multiple effect distillation

In the multiple effect distillation, the separation takes place in two different columns working at different pressures. This way the top stream of the column working at higher pressure is introduced in the heat exchanger as hot stream, and the one leaving the bottom of the lower pressure column enters as cold stream circulating at countercurrent. This way the hot stream condensates and the cold one is vaporized. The other streams are heated or cooled using a reboiler and a condenser respectively.

To optimize the process two conventional distillation columns are simulated. The feed stream (Feed_ME), with a pressure matching the low-pressure column (T-105-2), is divided in a tee (TEE-101) into two streams feeding each column. One of said streams enters a pump (P-100) that elevates the pressure to the required one. Both columns have their respective condensers and reboilers, and the number of stages is the previously determined with the shortcut method. The amount of heat exchanged this way is regulated with the flow ratios leaving the tee (TEE-101-2-2) using an adjust, that minimizes the difference between the duties of the high pressure column's condenser (Q-T1_Cond) and the duty of the low pressure column's reboiler (Q-T2_Reb). Said difference is calculated in a spreadsheet (SPRDSHT-3) were the values of the duties are imported.

When the flow ratios are optimized the columns are simulated using a reboiled absorber (T-109) as the high-pressure column and a refluxed absorber (T-108) as the low-pressure one. The bottom stream of the low-pressure column (7-2) enters the heat exchanger as cold fluid and then is separated into vapor and liquid streams, (17) and (18) respectively. The vapor is reintroduced into the bottom of the column as boilup and the liquid is mixed with the bottom stream of the high-pressure column (15) in a mixer (MIX-102) forming the stream with 50 kmoles/h of n-butane 90%.

The top stream of the high-pressure column (8-2) enters the hot side of the heat exchanger and condensates (10-2). Said steam is divided in the tee (TEE-102-2) to match the values of the reflux stream (4-2) and the recycle (RCY-3-2) is closed. The other stream leaving the tee (13-2) is mixed with the stream leaving the top of the low-pressure column (6-2) in the mixer (MIX-101) forming the stream with 50 kmoles/h of i-butane 90%.

To avoid problems when closing the loops, the streams entering and leaving the recycle are checked and the cycle is closed only if they match.

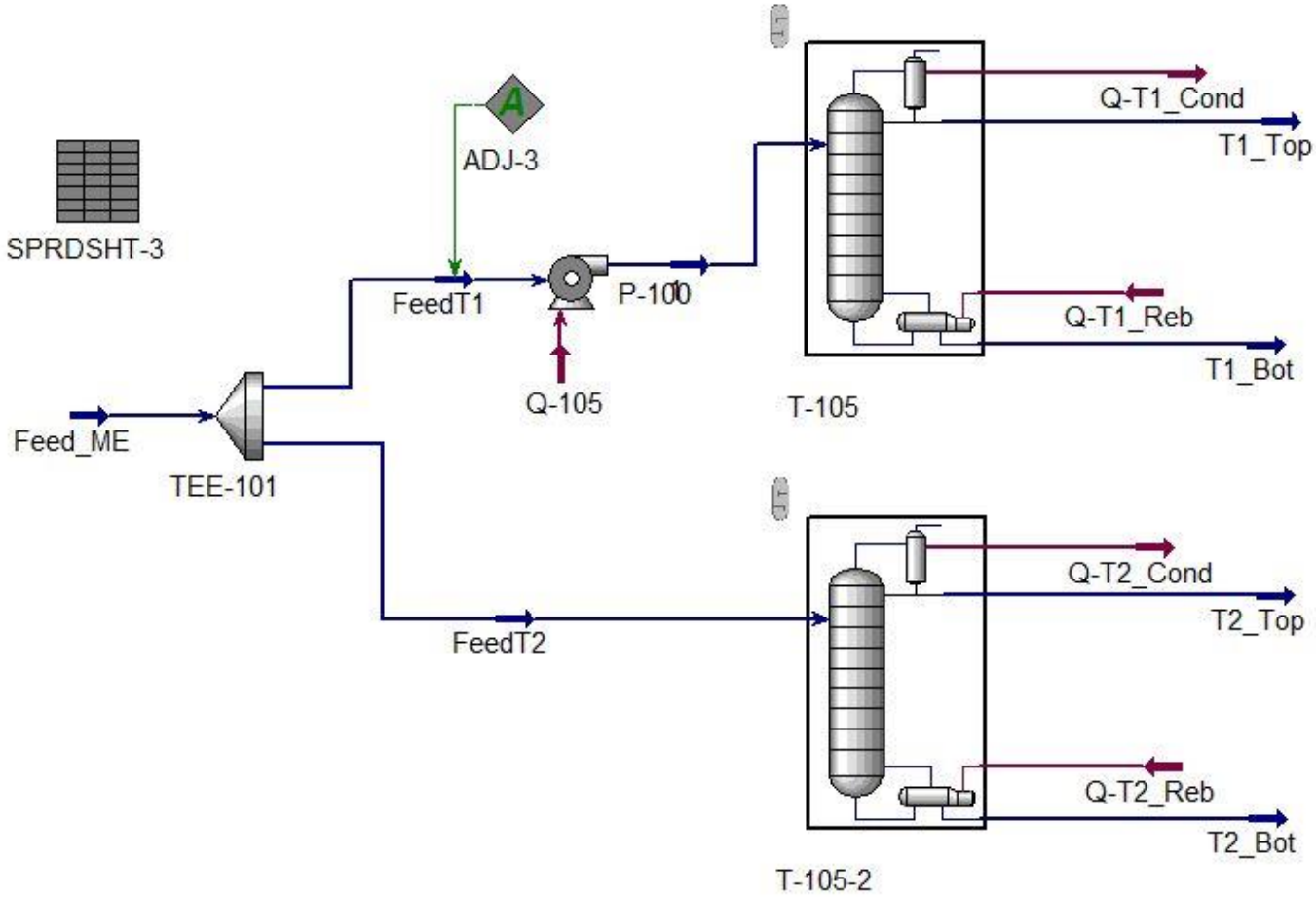

Figure 5.1. Process flow diagram of the multiple effect distillation.

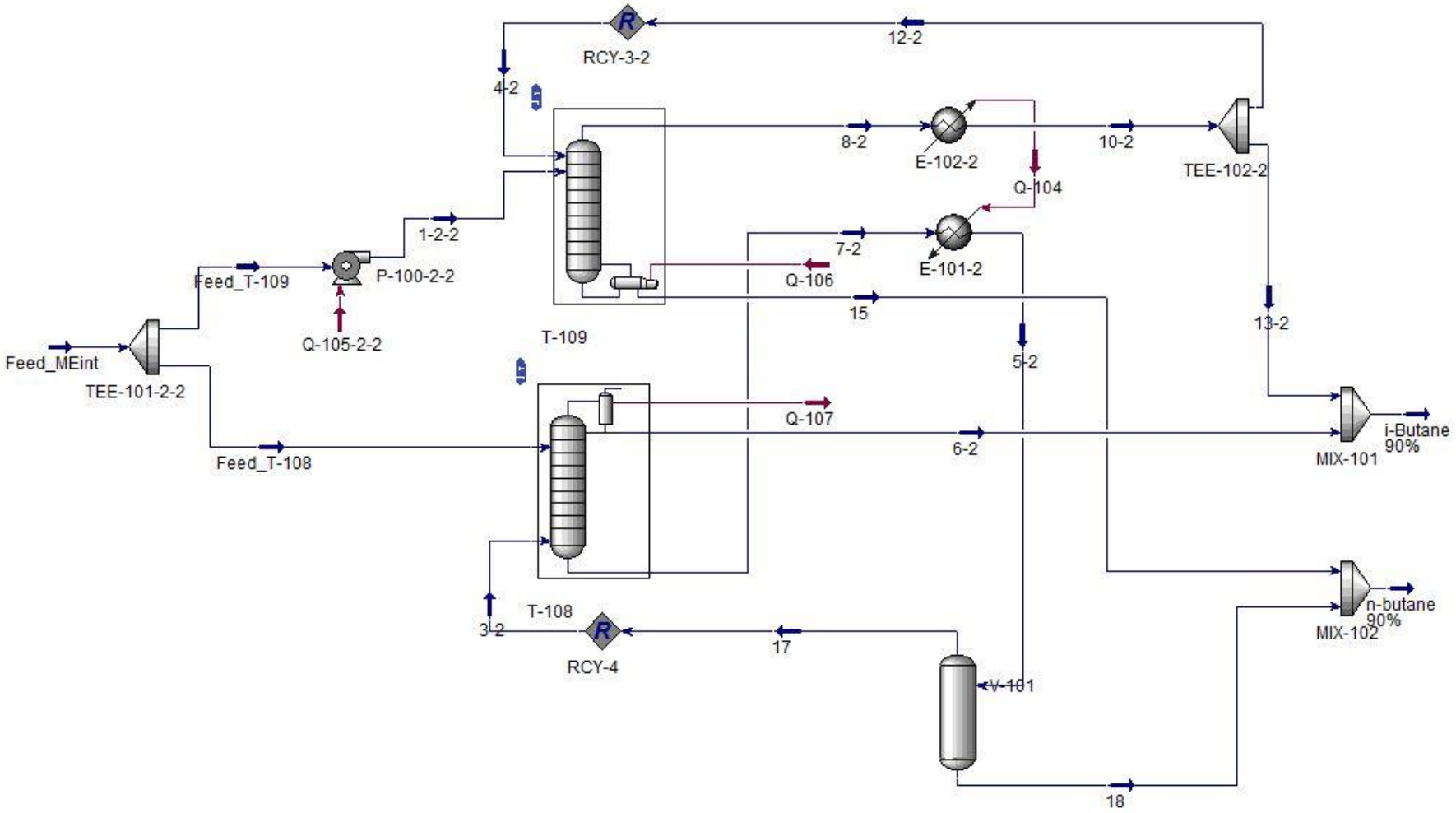

Figure 5.2. Process flow diagram of the multiple effect optimization with heat integration.

6 Results

Table 6.1. Annualized costs and power consumed in the different heat integration alternatives.

Alternative	Total Utilities Power Consumed (kJ/yr)	YOC ($/yr)	Annualized Equipment Cost ($/yr)	EAOC ($/yr)
CD	$1{,}426 \cdot 10^7$	$3{,}160 \cdot 10^5$	$7{,}765 \cdot 10^4$	$4{,}102 \cdot 10^5$
TVRHP	$2{,}062 \cdot 10^6$	$1{,}719 \cdot 10^5$	$2{,}081 \cdot 10^5$	$3{,}800 \cdot 10^5$
TBFHP	$1{,}862 \cdot 10^6$	$1{,}561 \cdot 10^5$	$1{,}613 \cdot 10^5$	$3{,}174 \cdot 10^5$
MED	$6{,}941 \cdot 10^6$	$1{,}525 \cdot 10^5$	$1{,}049 \cdot 10^5$	$2{,}656 \cdot 10^5$

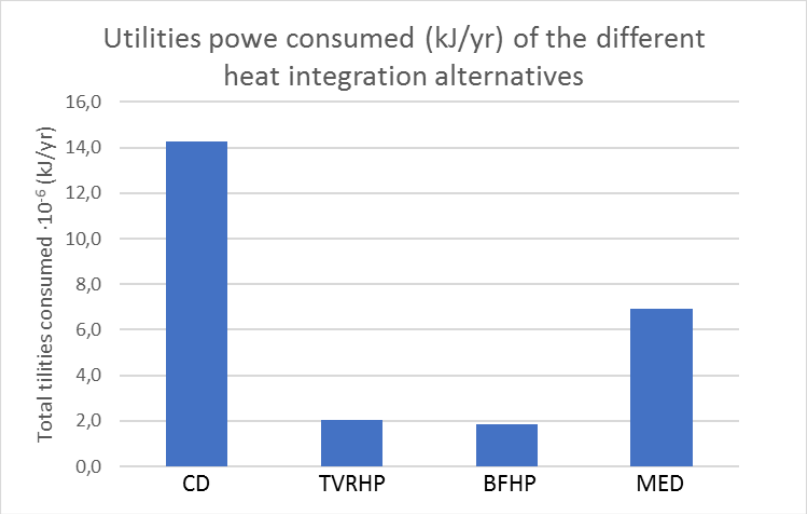

Figure 6.1. Total utilities consumed in the different heat integration alternatives.

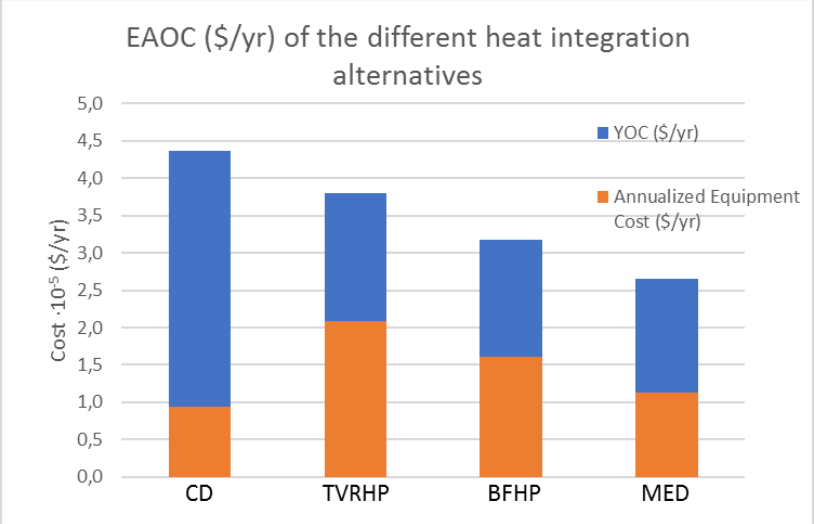

Figure 6.2. Annualized costs of the different heat integration alternatives.

The chosen column is the one that works at a pressure of 700 kPa and a reflux ratio of 1.3 times the minimum because it is the one that involves the smallest investment in equipment (8,441 · 10^4 \$/yr). This criterion counts on the reduction of the weight of the YOC once the power consumption is reduced balancing the importance of both equipment and utility cost. This also serves as a basis for comparing the heat integration alternatives with only one simulation each, reducing the time needed to carry the study.

With the mechanical heat pumps the utilities' power consumed is reduced from $1.426 \cdot 10^7$ kJ/yr in the conventional distillation to $2.062 \cdot 10^6$ kJ/yr when using the top vapor recompression heat pump (an 85.5%). With the bottom flashing heat pump, it is reduced even further to $1.862 \cdot 10^7$ kJ/yr (an 86.9%). However, the main energy source is electricity, which is four times more expensive than the low-pressure steam (4.54 \$/GJ vs 18.72 \$/GJ). That is the reason that even if the power used is reduced to a 14.5% of the original, the YOC is only reduced from $3.423 \cdot 10^5$ \$/yr to $1.719 \cdot 10^5$ \$/yr a 50% in the case of the TVRHP. With the BFHP with 13.1% of the original power usage the YOC is only reduced to $1.561 \cdot 10^5$ \$/yr (a 54.4%). On the other hand, with the multiple effect distillation, using the same kind of utilities as the conventional distillation, the energy of the utilities used are shorted by half to a 48.7% ($6.941 \cdot 10^6$ kJ/yr) of the original ones, reducing the YOC to $1.525 \cdot 10^5$ a 44.6% of the original.

In the case of the equipment cost, its value is doubled when using the TVRHP, increasing from $9.414 \cdot 10^4$ \$/yr to $2.081 \cdot 10^5$ \$/yr, a 221% of the original annualized equipment cost. Almost doubled in case of the BFHP, reaching $1.613 \cdot 10^5$ \$/yr (a 171%) and slightly increased in the case of the MED to $1.13 \cdot 10^5$ \$/yr (a 120% of the original). The main difference between the heat pumps and the MED is the use of a compressor, significantly more expensive than the rest of the equipment used. For example, in the TVRHP configuration the compressor has an updated bare module cost of $5.898 \cdot 10^5$ \$, while the second highest, the heat exchanger, is $1.377 \cdot 10^5$ \$. In the BFHP the problem is still the same, the compressor updated bare module cost is $5.442.10^5$ \$ while the heat exchanger is $9.529 \cdot 10^4$ \$.

The study can be taken further by integrating the heat at the top of the low-pressure column and the bottom of the high-pressure one. The issue with this line of research is that the temperature difference is not big enough to directly integrate the heat (the hot stream would be at 39.07 ºC and the cold one at 69.19 ºC making the condensation of the hot stream and the evaporation of the cold one infeasible. The work driven heat pumps are discarded because the EAOC reduction is not big enough to cover the indirect costs of increasing the complexity of the process. But this is a very interesting line of research for future projects.

When considering the use of other alternatives relying in electricity-powered utilities such as air coolers they can be discarded after seeing the impact of such elevated utility cost in the yearly operating cost of the process.

This makes the multiple effect distillation the best alternative, economically speaking. A reduction in the price of the electricity would increase the feasibility of the use of

compressors, since these options are the most efficient and less polluting when electricity is obtained from renewable sources.

7 Conclusion

The direct sizing of the equipment using HYSYS software was rejected since the complexity of the simulation increased drastically. Many attempts were made trying to use air cooled heat exchangers and shell and tube heat exchangers but the number of required adjusts to make the simulation converge maintaining all the energy and mass balances was of high inconvenience. A more simplistic approach was taken using heaters and coolers with shared energy streams and it turned of great use, the increase in simplicity brought a higher simulation speed allowing the implement of more varied configurations and requiring less adjusts.

Introducing all the parameters in the spreadsheet to apply the module factor approach was slow in the beginning but the automatization of the process accelerated the calculations in later simulations. Only requiring the modification of the imported parameters that could be sent to the spreadsheet directly from the process units' menu. This also worked when monitoring the process, because all the important information was displayed at the screen simultaneously.

Personally, this project has allowed me to appreciate the revolutionary advance that means use of specialized software that contains all the heuristic methods developed for years facilitating the job of the engineer that does not need to introduce all the equations by hand. However, I think that the research of those methods in the bibliography was key to understanding what I was accomplishing at every stage of the process unveiling the secrets of the previously perceived as mystic simulation, process stoking my curiosity and encouraging me to become a better chemical engineer.

APPENDIX A. CALCULATIONS

A.1 Estimation of capital cost

Equation A.1.1 is used to calculate the bare module cost of process units present in each case.

$$C_{BM} = C_p^o F_{BM} = C_p^o (B_1 + B_2 F_M F_P) \quad \text{(A.1.1)}$$

In this equation a standardized purchase cost of the equipment needed is represented by C_p^o and then it is adjusted with the bare module factors modifying the cost to resemble the one that the final equipment would have once installed to adjust to the working conditions. The bare module factor can be fixed, for compressors, or be calculated using coefficients B_1 and B_2, with different values for different types of process units, material factors (F_M) and pressure factors (F_P). Different equipment types have different material factors depending on the material used to craft them, the more expensive the material the higher the material factor, its values are found in table A.5 at Turton's [3]. F_P pressure factor is used to adjust the structural strength of different equipment types to be able to perform correctly under working pressure, and it is calculated using equation A.1.1.

First the purchase cost of the equipment working at ambient pressure and built in carbon steel (C_p^o) is calculated using equation A.1.2.

$$Log_{10}(C_p^o) = K_1 + K_2\, Log_{10}(A) - K_3\, [Log_{10}(A)]^2 \quad \text{(A.1.2)}$$

Were K_i being coefficients characteristic for each equipment type and A is the sizing variable specific for that equipment. Values required in each simulation are compiled in fables B.1 to B.3.

In second place, F_{BM} is applied. In this case it is fix for the compressors, registered in figure A.19 at Turton's [3], and calculated for the rest of equipment using equation A.1. 1.

The constants for bare module factor B1 and B2, as well as the material factor are found in the bibliography, tables A.4 and A.5 respectively. The pressure factor is calculated using equation A.1.3 using the pressure in gauge bars and the corresponding coefficients found in table A.2[3]. Except for the process vessels, including distillation tower vessels, for those, equation A.1.4 is used.

$$Log_{10}(F_P) = C_1 + C_2\, Log_{10}(P) - C_3\, [Log_{10}(P)]^2 \quad \text{(A.1.3)}$$

$$F_{P,vessel} = \frac{\frac{PD}{2[850]-0.6(P)} + 0{,}00315}{0{,}0063} \quad \text{(A.1.4)}$$

The equation used to calculate the bare module cost of the trays is different, equation A.1.5. Were N being the number of trays inside the distillation column and F_q being a quantity factor for trays calculated with equation A.1.6 if N is lower than 20, else F_q equals 1.

$$C_{BM} = C_p^o \, N \, F_{BM} \, F_q \qquad \text{(A.1.5)}$$

$$Log_{10}(F_q) = 0{,}4771 + 0{,}08516 \, Log_{10}(N) \, - 0{,}3473 \, [Log_{10}(N)]^2 \qquad \text{(A.1.6)}$$

Once calculated the Bare Module Factor the results must be updated.

To update the cost of the equipment equation A.1.6 is used adjusting the values of the purchased equipment from 2001 to 2019. "*All the data for the purchased cost of equipment for the second edition of this book were obtained from a survey of equipment manufacturers during the period May to September of 2001, so an average value of the CEPCI of 397 over this period should be used when accounting for inflation."*[3]

$$Cost_2 = \frac{CEPCI_2}{CEPCI_1} Cost_1 \qquad \text{(A.1.6)}$$

$CEPCI_1$ is 397, the $CEPCI_2$ is the one of the second semester of 2019[8]. And $Cost_2$ is for the updated cost and $Cost_1$ the one calculated with the provided coefficients.

Finally, the cost is converted to euros per year. The conversion factor to calculate the cost in €/yr is 0.9393 €/$. This factor is the average of the second semester of 2019.

A.2 Calculating the area of the heat exchangers

The heat exchangers used in this study consist roughly of devices were a hot fluid transmits heat through a wall to a cold one.

To calculate the area of heat exchange equation A.2.1 is used:

$$Q = U_o A_o \Delta T_{LM} F_o = U_I A_I \Delta T_{LM} F_I \qquad (A.\,2.1)$$

When using this equation steady state is considered, therefore the heat flow in the inner side of the wall equals the heat flow in the outer side.

Q represents the heat flow. U is the overall heat transfer coefficient, calculated using equation A.2.4. A is the effective heat transfer area. ΔT_{LM} is the logarithmic mean of the temperatures in both extremes of the heat exchanger. This parameter corrects the non-linearity of the temperature profile inside and outside the wall avoiding this way the need to know the function that those profiles follow and introduce them in equation (A.2.2) Finally, F is the fouling factor, represents the increment of the heat resistance of the wall due to the formation of sediments. The fouling factor is not considered in the calculus, so F=1.

The temperature profile inside the heat exchangers have a similar form of the one showed in figure A.2.1. were 1 is be the part of the heat exchanger were the hot stream enters and 2 were it leaves. All heat exchangers are considered to wok counter flow and all temperature differences are positives.

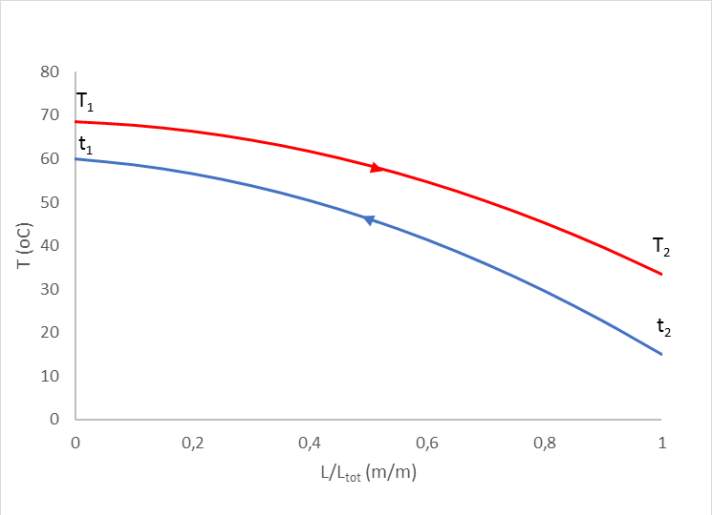

Figure A.2.1. Example of temperature profile inside a heat exchanger.

$$\Delta T_{LM} = \frac{\Delta T_1 - \Delta T_2}{Ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} \qquad (A.2.2)$$

Q is calculated automatically by HYSYS solving an energy balance, ΔT_{LM} is calculated in a spreadsheet using the values of the outlet and inlet streams to the heat exchanger. If the temperature remains constant, along the inner or outer side the temperature profile is considered lineal and is calculated using simply equation (A.2.3)

$$\Delta T_{LM} = \Delta T_1 - \Delta T_2 \qquad (A.2.3)$$

$$U = \left[\frac{1}{D_o} + \frac{D_o\, Ln(D_o/D_i)}{2k_w} + \frac{D_o}{D_i} + \frac{D_o}{D_i}\frac{1}{h_i}\right]^{-1} \qquad (A.2.4)$$

k_w is the tube material conductivity (in W/m K) and is equal to 45,4 (the average for carbon steel between 0 ºC and 100 ºC)[9] h is the film transfer coefficient (in W/m^2 K) and its values are registered in table A.2.1. D is the tube diameter, being external (o) or internal (i).

Table A.2.1. Values of the film heat transfer coefficient[10].

	h (J/s m2 K)
Condensed vapor	$5{,}675 \cdot 10^3$
Vaporizing liquid	$2{,}840E \cdot 10^3$
Process liquid stream	$5{,}675 \cdot 10^3$
Process vapor stream	$5{,}675 \cdot 10^3$
Cooling water	$5{,}675 \cdot 10^3$

A.3 Yearly Operating Cost

To calculate the yearly operational cost the cost of the utilities is considered to be provided by Off-Sites for the same plant with Multiple Process Units: "*Cost Represents Charges for Utilities Delivered to the Battery Limit of a Process and Are Based on the Natural Gas Cost and Electricity Price Listed in This Table*" Richard Turton. Analysis Synthesis and Design of Chemical Processes. 2018: 245-.247.

The data required to calculate the YOC of the heat integration alternatives used in this study is contained in table A.3.1 and later in tables B1 to B.4.

Table A.3.1. Utilities Provided by OFF-Sites for a Plant with Multiple Process Units

Utility	Description	Cost ($/GJ)
Steam from Boilers	Process steam: latent heat only. Low pressure (5 barg, 160°C) form HP steam without credit for power	4,54
Cooling Tower Water	Process cooling water: 30°C to 40°C of 45°C	0,378
Electrical Substation	Electric Distribution	18,72

APPENDIX B. RESULTS OF THE CAPITAL COST OF THE STUDIED ALTERNATIVES

Table B.1 EAOC of the conventional distillation process. R/R_{min}= 1,3 and P_{Top} = 700 kPa.

Label	**Main Tower**		**Condenser**	**Reboiler**
Equipment Type	Process Vessel	Trays	Heat exchanger	Heat exchanger
Equipment Description	Vertical	Sieve	Floating head	Kettle reboiler
Fixed Costs				
Parameter A	17.67	0.8759	52.29	20.18
Capacity, units	Volume, m^3	Area, m^2	Area, m^2	Area, m^2
K_1	3.497	2.995	4.831	4.4646
K_2	0.4485	0.4465	-0.8509	-0.5277
K_3	0.1074	0.3961	0.3187	0.3955
C_p^o ($)	$1.675 \cdot 10^4$	934.6	$2.039 \cdot 10^4$	$2.815 \cdot 10^5$
Pressure (barg)	6.187	-	5.987	6.187
D	1.128	-	-	-
C_1	-	-	0.03881	0.03881
C_2	-	-	-0.1127	-0.1127
C_3	-	-	0.08183	0.08183
F_P	1.155	-	1	1
F_M	1	-	1.375	1.375
B_1	2.25	-	1.63	1.63
B_2	1.82	-	1.66	1.66
F_{BM}	4.351	1	3.912	3.912
N	-	33	-	-
F_q	-	1	-	-
C_{BM} ($) (2001)	$7.286 \cdot 10^4$	$3.084 \cdot 10^4$	$7.979 \cdot 10^4$	$1.101 \cdot 10^5$
C_{BM} ($) (2019, S2)	$1.115 \cdot 10^5$	$4.719 \cdot 10^4$	$1.221 \cdot 10^5$	$1.685 \cdot 10^5$

Label	**Main Tower**		**Condenser**	**Reboiler**
Variable Costs				
Power Consumed (kJ/h)	-	-	$7.131 \cdot 10^6$	$7.126 \cdot 10^6$
Utility	-	-	Cooling Tower Water	Low Pressure Steam
Description	-	-	30 °C to 40 °C	5 barg 160 °C,
Cost ($/GJ)	-	-	0.378	4.54
Operating Cost ($/h)	-	-	2.694	36.14
YOC ($/yr)	-	-	$2.362 \cdot 10^4$	$3.160 \cdot 10^5$
Total Cost				
Total C_{BM} ($) (2019, S2)	$4.493 \cdot 10^5$			
Annuity Factor (yr^{-1})	0.2			
YOC ($/yr)	$3.423 \cdot 10^5$			
EAOC ($/yr)	$4.364 \cdot 10^5$			
EAOC (€/yr) (2019 S2)	$4.099 \cdot 10^5$			

TableB.2. Cost of the process with a Top Vapor Recompression Heat Pump

Label	**T-104**		**K-101**	**Tube_TVRHP**	**E-100**	**V-100**
Equipment Type	Process Vessel	Trays	Compressor	Heat exchanger	Heat exchanger	Process vessel
Equipment Description	Vertical	Sieve	Centrifugal	Fixed Tube	Fixed tube	Vertical
Fixed Costs						
Parameter A	20,12	0.8762	285.1	89.86	5.602	4.982
Capacity, units	Volume, m^3	Area, m^2	Fluid power, kW	Area, m^2	Area, m^2	Volume, m^3
K_1	3.497	2.995	3.205	4.325	4.325	3.497
K_2	0.4485	0.4465	0.7468	-0.3030	-0.3030	0.4485
K_3	0.1074	0.3961	0.00651	0.1634	0.1634	0.1074
C_p^o ($)	$1.675 \cdot 10^4$	934.7	$1.195 \cdot 10^5$	$2.273 \cdot 10^4$	$1.548 \cdot 10^4$	7285
Pressure (barg)	6.187	-	-	15.85	15.85	6.187
D	1.128	-	-	-	-	1.219
C_1	-	-	-	-0.001640	-0.001640	-
C_2	-	-	-	-0.00627	-0.00627	-
C_3	-	-	-	0.0123	0.0123	-
F_P	1.155	-	-	1.02	1.02	1.207
F_M	1	-	-	1.375	1.375	1
B_1	2.25	-	-	1.63	1.63	2.25
B_2	1.82	-	-	1.66	1.66	1.82
F_{BM}	4.351	1	2.6	3.958	3.958	1
N	-	33	-	-	-	-
F_q	-	1	-	-	-	-
C_{BM} ($) (2001)	$7.288 \cdot 10^4$	$3.084 \cdot 10^4$	$3.107 \cdot 10^5$	$8.998 \cdot 10^4$	$6.126 \cdot 10^4$	$3.24 \cdot 10^4$
C_{BM} ($) (2019, S2)	$1.115 \cdot 10^5$	$4.719 \cdot 10^4$	$5.895 \cdot 10^5$	$1.377 \cdot 10^5$	$9.375 \cdot 10^4$	$4.958 \cdot 10^4$

Label	T-104		K-101	Tube_TVRHP	E-100	V-100
Variable Costs						
Power Consumed (kJ/h)	-	-	$1.026 \cdot 10^6$	-	$1.035 \cdot 10^6$	-
Utility	-	-	Electrical Substation	-	Cooling Tower Water	-
Description	-	-	Electric Distribution	-	30 °C to 40 °C	-
Cost ($/GJ)	-	-	18.72	-	0.378	-
Operating Cost ($/h)	-	-	19.22	-	0.3914	-
YOC ($/yr)	-	-	$1.685 \cdot 10^5$	-	3432	-
Total Cost						
Total C_{BM} ($) (2019, S2)	$1.040 \cdot 10^6$					
Annuity Factor (yr^{-1})	0.2					
YOC ($/yr)	$1.719 \cdot 10^5$					
EAOC ($/yr)	$3.800 \cdot 10^5$					
EAOC (€/yr) (2019 S2)	$3.569 \cdot 10^5$					

TableB.3. Cost of the process with a Bottom Flashing Heat Pump

Label	**T-104**		**K-101***	**Tube_BFHP**	**E-100**	**V-100**
Equipment Type	Process Vessel	Trays	Compressor	Heat exchanger	Heat exchanger	Process vessel
Equipment Description	Vertical	Sieve	Centrifugal	Fixed Tube	Fixed tube	Vertical
Fixed Costs						
Parameter A	20,12	0.8762	259,0	82,85	4,044	4,982
Capacity, units	Volume, m^3	Area, m^2	Fluid power, kW	Area, m^2	Area, m^2	Volume, m^3
K_1	3.497	2.995	3.205	4.325	4.325	3.497
K_2	0.4485	0.4465	0.7468	-0.3030	-0.3030	0.4485
K_3	0.1074	0.3961	0.00651	0.1634	0.1634	0.1074
C_p^o ($)	$1.839 \cdot 10^4$	934.7	$1,103 \cdot 10^5$	$2,213 \cdot 10^4$	$1.590 \cdot 10^4$	7285
Pressure (barg)	6.187	-	-	5,987	6,187	6.187
D	1.128	-	-	-	-	1.219
C_1	-	-	-	-0.001640	-0.001640	-
C_2	-	-	-	-0.00627	-0.00627	-
C_3	-	-	-	0.0123	0.0123	-
F_P	1.155	-	-	1.02	1.02	1.207
F_M	1	-	-	1.375	1.375	1
B_1	2.25	-	-	1.63	1.63	2.25
B_2	1.82	-	-	1.66	1.66	1.82
F_{BM}	4.351	1	2.6	3.958	3.958	1
N	-	33	-	-	-	-
F_q	-	1	-	-	-	-
C_{BM} ($) (2001)	$8,002 \cdot 10^4$	$3.084 \cdot 10^4$	$2,867 \cdot 10^5$	$8.670 \cdot 10^4$	$6,227 \cdot 10^4$	$3,240 \cdot 10^4$
C_{BM} ($) (2019, S2)	$1.224 \cdot 10^5$	$4.719 \cdot 10^4$	$5.442 \cdot 10^5$	$1.327 \cdot 10^5$	$9.529 \cdot 10^4$	$4.958 \cdot 10^4$

Label	T-104		K-101	Tube_BFHP	E-100	V-100
Variable Costs						
Power Consumed (kJ/h)	-	-	$9{,}394 \cdot 10^5$	-	$9.292 \cdot 10^5$	-
Utility	-	-	Electrical Substation	-	Cooling Tower Water	-
Description	-	-	Electric Distribution	-	30 °C to 40 °C	-
Cost ($/GJ)	-	-	18.72	-	0.378	-
Operating Cost ($/h)	-	-	17,46	-	0,3513	-
YOC ($/yr)	-	-	$1{,}53 \cdot 10^5$	-	3079	-
Total Cost						
Total C_{BM} ($) (2019, S2)	$8.588 \cdot 10^5$					
Annuity Factor (yr^{-1})	0.2					
YOC ($/yr)	$1.561 \cdot 10^5$					
EAOC ($/yr)	$3{,}174 \cdot 10^5$					
EAOC (€/yr) (2019 S2)	$2.982 \cdot 10^5$					

*The compressor's coefficients are taken from G.E. Garret's Chemical Engineering Economics. 1989: Apendix A[11]. The reason: the value of the fluid power obtained was out the range usable for the compressors compiled by Turton . Therefore, the CEPCI is the one form 1989, 320.

Table B.4. Multiple effect distillation

Label	**T-109**			**P-100-2-2**	**E-102-2**	**V-101**
Equipment Type	Process Vessel	Trays	Heat exchanger	Pump	Heat exchanger	Process vessel
Equipment Description	Vertical	Sieve	Kettle Reboiler	Reciprocating	Fixed tube	Vertical
Fixed Costs						
Parameter A	10.14	0.4109	6.721	0.5808	77.62	2.102
Capacity, units	Volume, m^3	Area, m^2	Area, m^2	Shaft power, kW	Area, m^2	Volume, m^3
K_1	3.497	2.995	4.465	3.867	4.325	3.497
K_2	0.4485	0.4465	-0.5277	0.3161	-0.3030	0.4485
K_3	0.1074	0.3961	0.3955	0.1220	0.1634	0.1074
$C_p^o \cdot (\$)$	$1.141 \cdot 10^4$	934.7	$1.989 \cdot 10^4$	6336	$2.168 \cdot 10^4$	4500
Pressure (barg)	7.187	-	7.187	7.087	6,187	4.187
D	1.128	-	-	-	-	1.219
C_1	-	-	0.03881	-02454	-0.001640	-
C_2	-	-	-0.1127	0.2590	-0.00627	-
C_3	-	-	0.0497	-0.01363	0.0123	-
F_P	1.025	-	1	1	1.004	1
F_M	1	-	1.375	1.65	1.375	1
B_1	2.25	-	1.630	1.89	1.63	2.25
B_2	1.82	-	1.660	1.35	1.66	1.82
F_{BM}	4.115	1	3.803	4.117	3.922	1
N	-	35	-	-	-	-
F_q	-	1	-	-	-	-
C_{BM} *(\$) (2001)*	$8{,}002 \cdot 10^4$	$2.665 \cdot 10^4$	$7.567 \cdot 10^4$	$2.609 \cdot 10^4$	$8.502 \cdot 10^4$	$1.832 \cdot 10^4$
C_{BM} *(\$) (2019, S2)*	$4.695 \cdot 10^4$	$4.719 \cdot 10^4$	$1.158 \cdot 10^5$	$3.992 \cdot 10^4$	$1.301 \cdot 10^5$	$2.03 \cdot 10^4$

Label	**T-109**			**P-100-2-2**	**E-102-2**	**V-101**
Variable Costs						
Power Consumed (kJ/h)	-	-	$3.541 \cdot 10^6$	$2.091 \cdot 10^3$	-	-
Utility	-	-	Low Pressure Steam	Electrical Substation	-	-
Description	-	-	5 barg 160 ^oC,	Electric Distribution	-	-
Cost ($/GJ)	-	-	4.54	18.72	-	-
Operating Cost ($/h)	-	-	9.844	$3.914 \cdot 10^{-2}$	-	-
YOC ($/yr)	-	-	$1,409 \cdot 10^5$	343.1	-	-

Label	**T-108**		
Equipment Type	Process Vessel	Trays	Heat exchanger
Equipment Description	Vertical	Sieve	Floating head
Fixed Cost			
Parameter A	8.616	0.4172	42.05
Capacity, units	Volume, m^3	Area, m^2	Area, m^2
K_1	3.497	2.995	4.831
K_2	0.4485	0.4465	-0.8509
K_3	0.1074	0.3961	0.3187
$C_p^o \cdot (\$)$	$1.025 \cdot 10^4$	763.1	$1.946 \cdot 10^4$
Pressure (barg)	4.187	-	3.987
D	0,7745	-	-
C_1	-	-	0.03881
C_2	-	-	-0.1127
C_3	-	-	0.08183
F_P	1	-	1

F_M	1	-	1.375
B_1	2.25	-	1.63
B_2	1.82	-	1.66
F_{BM}	4.351	1	3.912
N	-	30	-
F_q	-	1	-
C_{BM} ($) (2001)	$4.173 \cdot 10^4$	$2.289 \cdot 10^4$	$7.505 \cdot 10^4$
C_{BM} ($) (2019, S2)	$6.385 \cdot 10^4$	$3.503 \cdot 10^4$	$1.148 \cdot 10^5$
Variable Costs			
Power Consumed (kJ/h)	-	-	$3.398 \cdot 10^6$
Utility	-	-	Cooling Tower Water
Description	-	-	30 °C to 40 °C
Cost ($/GJ)	-	-	0.378
Operating Cost ($/h)	-	-	1.284
YOC ($/yr)	-	-	$1.24 \cdot 10^4$
Total Cost			
Total C_{BM} ($) (2019, S2)	$5.652 \cdot 10^5$		
Annuity Factor (yr^{-1})	0.2		
YOC ($/yr)	$1.525 \cdot 10^5$		
EAOC ($/yr)	$2.656 \cdot 10^5$		
EAOC (€/yr) (2019 S2)	$2.495 \cdot 10^5$		